

Supplement Search

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Page 1

=> file registry

FILE 'REGISTRY' ENTERED AT 10:54:12 ON 02 DEC 2002

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 1 DEC 2002 HIGHEST RN 474745-06-7

DICTIONARY FILE UPDATES: 1 DEC 2002 HIGHEST RN 474745-06-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

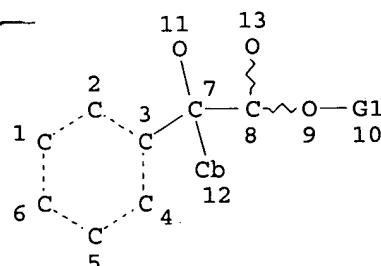
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STN Note 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> d que l8

L1 STR



Ak @14

VAR G1=H/14

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 11

CONNECT IS E1 RC AT 13

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS E6 C AT 12

ECOUNT IS M1-X15 C AT 14

GRAPH ATTRIBUTES:

RSPEC I

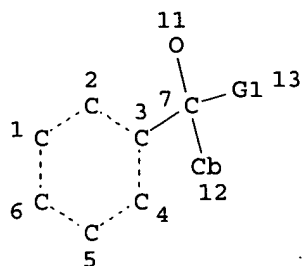
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L2 2026 SEA FILE=REGISTRY SSS FUL L1

L3 STR

I realized that I made an error on the initial structure. When $G_1 = H$ it will not allow for acids (due to the way CA indexes them) because of the bond between the $O@9$ & $G_1@10$. So I tried the search with the structure L3 on the following page...



VAR G1=15/18
 NODE ATTRIBUTES:
 CONNECT IS E1 RC AT 11
 CONNECT IS E1 RC AT 16
 CONNECT IS E1 RC AT 21
 CONNECT IS E1 RC AT 22
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED
 ECOUNT IS E6 C AT 12
 ECOUNT IS M1-X15 C AT 20

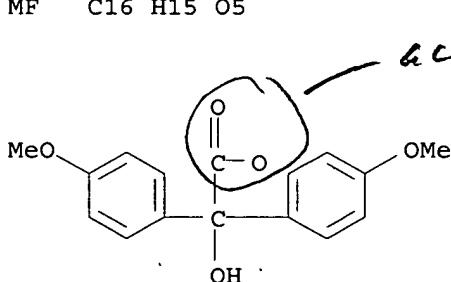
GRAPH ATTRIBUTES:
 RSPEC I
 NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE

L7 2031 SEA FILE=REGISTRY SSS FUL L3
 L8 5 SEA FILE=REGISTRY ABB=ON PLU=ON L7 NOT L2

=> d scan

L8 5 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN Ethoxy, 2-hydroxy-2,2-bis(4-methoxyphenyl)-1-oxo- (9CI)
 MF C16 H15 O5



This structure allows for esters, Ak is defined as before.

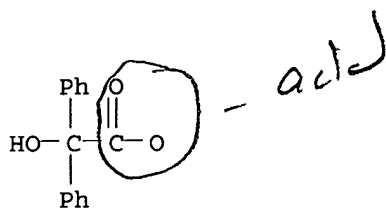
This structure allows for carboxylic acids whether the counter ion is H^+ or a metal ion.

← 5 more structures were picked up with L3 vs L1 used in original search.

Both cyclic groups are aromatic, not saturated or with one double bond.

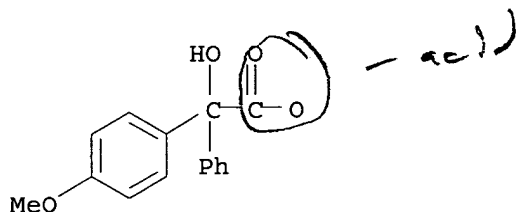
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L8 5 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN Ethoxy, 2-hydroxy-1-oxo-2,2-diphenyl- (9CI)
 MF C14 H11 O3



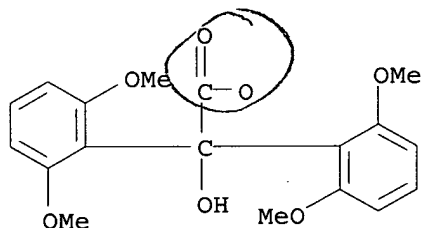
both rings aromatic

L8 5 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN Ethoxy, 2-hydroxy-2-(4-methoxyphenyl)-1-oxo-2-phenyl- (9CI)
 MF C15 H13 O4



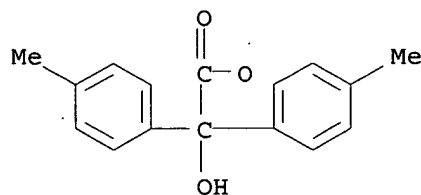
both rings aromatic
 MW

L8 5 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN Ethoxy, 2,2-bis(2,6-dimethoxyphenyl)-2-hydroxy-1-oxo- (9CI)
 MF C18 H19 O7



2 aromatic rings
 MW

L8 5 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN Ethoxy, 2-hydroxy-2,2-bis(4-methylphenyl)-1-oxo- (9CI)
 MF C16 H15 O3



2 aromatic rings
 MW

ALL ANSWERS HAVE BEEN SCANNED

∴ None of the new answers appears to meet the limitations of the claimed structure.

Searched by Thom Larson, STIC, 308-7309